

## **Local resolution of the particle shape in DEM-CFD for more accurate cost-effective simulations of moving reacting packed beds**

Max Brömmner<sup>1</sup>, Enric Illana<sup>1\*</sup>, Viktor Scherer<sup>1</sup>

\*lead presenter: [illana@leat.rub.de](mailto:illana@leat.rub.de)

<sup>1</sup> Chair of Energy systems and energy process technology, Germany

The shape of the particles in a reacting packed bed has an influence on the structure of the interstices between the particles, the resistance of the particles to flow and their reaction rate. In the DEM-CFD simulations of such systems, resolved methods like [1,2] consider the actual shape of the particles as well as the void spaces between them. The DEM side computes the bed structure and its movement, tracking the evolution of the actual particles, while on the CFD side solves the flow field around those particles. On the other hand, unresolved methods are computationally more cost-effective since the shape of the particles is modelled. The DEM assumes simplified particle shape, with effective material/contact parameters, while the bed is represented by a porosity field in the CFD [3].

While unresolved methods are accurate in regions where gradients are low, they are not well suited for regions where high gradients take place. Hence, advantage of local resolution arises as a compromise between accuracy and computational cost. In previous work [4], particles were represented in DEM as spheres except at predefined spatial zone, where the actual particle shape was used. Similarly, in [5] the porous media approach was applied in the whole domain except at a region near the inlet of a jet in cross flow, where the flow inside the interstices was computed.

In the present work, the local resolution concept has extended to the intraparticle models. The unresolved approach corresponds to a 1D radial solution while the resolved method uses a tetrahedral discretization. The transition between the models involves mapping the solution while enforcing the conservation of energy and species. The model is tested for different boundary conditions and compared with the fully resolved solution. Subsequently, a generic shaft is simulated with the combined local resolution methods and the accuracy and computational effort is assessed.

### **References**

- [1] A fast contact detection algorithm for 3-D discrete element method. *Computers and Geotechnics*. 2004;31:575-587.
- [2] Mittal R and Iaccarino G. Immersed Boundary Methods. *Annual Review of Fluid Mechanics*. 2005;37:239-261.
- [3] Wang L et al. Volume-averaged macroscopic equation for fluid flow in moving porous media. *International Journal of Heat and Mass Transfer*. 2015;82:357-368.
- [4] Illana E et al. Shape-changing particles for locally resolved particle geometry in DEM simulations. *Particuology*. 2024;89:185-190.
- [5] Illana E et al. Locally resolved simulation of gas mixing and combustion inside static and moving particle assemblies. *Chemical Engineering and Technology*. 2023;46:1362-1372.